

Algebraic solution for a two-level atom in radiation fields and the Freeman resonances

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(Received 3 October 2005; published 17 February 2006)

Using techniques of complex analysis in an algebraic approach, we solve the wave equation for a two-level atom interacting with a monochromatic light field exactly. A closed-form expression for the quasienergies is obtained, which shows that the Bloch-Siegert shift is always finite, regardless of whether the original or the shifted level spacing is an integral multiple of the driving frequency ω . We also find that the wave functions, though finite when the original level spacing is an integral multiple of ω , become divergent when the intensity-dependent shifted energy spacing is an integral multiple of the photon energy. This result provides an *ab initio* theoretical explanation for the occurrence of the Freeman resonances observed in above-threshold ionization experiments.

DOI: [10.1103/PhysRevA.73.023419](https://doi.org/10.1103/PhysRevA.73.023419)

PACS number(s): 32.80.Rm

I. INTRODUCTION

The interaction between light and matter is a fundamental problem in physics, whose study led to the birth of quantum theory about a century ago. The two-level atom model was originally proposed by Einstein [1] to study the transitions between two energy levels of an atom interacting with light (later especially with laser light). However, despite many great efforts and significant progress since then, an exact solution remains elusive even for the simplest problem of a two-level atom [2] interacting with a classical or quantum-mechanical light field. Pursuing higher accuracy in describing a physical system is always an ultimate goal for physicists.

Exact and analytic expressions also provide new starting points for further developments of the theories in physics. The exact quasienergy levels and the wave functions obtained by solving the two-level atom model can be used in the calculation of many important physical quantities, such as the Rabi flopping frequency and the inversion rate. Mathematically, an approach that exactly solves this model may provide a starting point for solving more complicated cases, such as a driven N -level atom, as well as an atom in a multimode laser field.

Since the pioneering work of Bloch and Siegert (BS) [3], there have been many different approximate methods developed to solve a two-level system driven by an external field. The rotating-wave approximation (RWA) is a widely used method. As is well known, this approximation is good only when the frequency of the light field is “near resonance” but also not too close to the resonance. The word “near” means that the frequency of the light field is near the original energy spacing of the two-level atom. Many works have been devoted to going beyond the RWA method. For example, Shirley [4] applied Floquet’s theorem and perturbation method to solve the time-dependent Schrödinger equation for a two-

level system. And Cohen-Tannoudji *et al.* [5] used perturbation methods to solve a quantum-field two-level system. Piazza *et al.* [6] have recently derived the wave functions and quasienergies for a two-level atom driven by a low-frequency strong laser pulse and applied their result to emission spectra and high harmonic generation (HHG). The low-frequency approximation adopted by Piazza *et al.* skips all higher resonances and can be thought of as a limiting case opposite to the near-resonance approximation. The continued fraction (CF) method, giving recurrence relations for the Fourier coefficients of the wave function, is also a commonly adopted method going beyond the RWA. Swain [7], Yeh and Stehle [8], Becker [9], and recently Feng *et al.* [10] applied the CF method to obtain approximate solutions. In continued fractions expressing the wave function, an unknown quasienergy is involved. Approximations, used in evaluating the quasienergy, make the corresponding wave functions inaccurate. Due to the infinite order of the algebraic equations satisfied by the quasienergy, the exact value of the quasienergy in a closed form has never been derived.

In 1987, Freeman *et al.* found experimentally [11] that the above-threshold ionization (ATI) peaks broke up into many small peaks when the laser pulses were short. The appearance of the small peaks was interpreted as multiphoton resonances between the ground state—say, $5P_{3/2}$ for the outermost shell electrons of xenon atoms—and Rydberg states with a shifted energy level. In the literature these resonances are now called Freeman resonances and their appearance can be phenomenologically explained by ac Stark-shifted multiphoton resonances.

Such multiphoton resonances have been observed for years and modeled theoretically using Floquet and numerical approaches [12]. Due to interactions with the radiation field, the energy-level spacing of a two-level atom acquires an intensity-dependent shift. In the theoretical literature, the term “near resonance” refers to the condition where the pho-

ton energy is near the original energy spacing (preresonances, in the absence of radiation). However, the fine structure of ATI peaks observed by Freeman *et al.* [11] can be well interpreted as Rydberg-state resonances occurring only when the shifted energy spacing is equal to an integral multiple of the photon energy, the Freeman resonances, in the presence of strong radiation fields. It is this intensity-dependent shift in the resonance frequency that calls for a fundamental explanation in the theory for a driven atom. Moreover, one is certainly tempted to know what happens when the light field is neither very near nor very far away from any resonance. Even in the so-called near-resonance case, calculations and analysis with higher accuracy are always desired. All of these require a solution to the two-level atom problem that is as exact as possible.

In this paper, we attack the two-level atom problem in an algebraic approach. We start with a proof of the equivalence between a classical-field description and a corresponding quantum-field description for a two-level system in a driving field. Then, we recast the classical-field differential equations of motion into an infinite system of linear equations, with the energy determinant of infinite rank in the form of a continuant [13]—i.e., having nonzero elements only on three major diagonals. We then directly evaluate the energy determinant, using techniques in complex analysis and the trick that breaks the relevant continuants into subcontinuants of a half-infinite rank, which are further expressed as infinite series. In this way, a closed-form expression for the quasienergies is obtained.

Our solutions exhibit several interesting features: (i) A simple cosine energy shift formula is derived, which naturally exhibits the Floquet quasienergy feature. (ii) It incorporates multiphoton effects, in particular all multiphoton resonances if there are any. (iii) For the preresonance cases, when the original energy spacing is an integral multiple of the photon energy of the radiation field, both the shifted quasienergies and the corresponding wave functions are finite. Therefore no singularity (or resonance) really appears at the preresonances. (iv) It shows theoretically the existence of Freeman resonances; namely, the wave function has a singularity when the intensity-dependent energy spacing shifts to an integral multiple of the external photon energy.

Comparisons made between our result and earlier results indeed show agreement at the leading order. The higher-order correctness of our results can be guaranteed and checked by the mathematical derivation process and also by a comparison with experimental findings.

II. EQUATIONS OF MOTION

The goal of this paper is to solve the following equations of motion which describe a two-level atom driven by a radiation field:

$$\left(\frac{d}{d\tau} - iD \cos \tau \sigma_x + i\Delta \sigma_z + iEI \right) \mathbf{Y} = 0. \quad (1)$$

In this equation, we have chosen $c = \hbar = 1$ and set the field frequency $\omega = 1$. Here 2Δ stands for the energy spacing in

units of ω in the absence of the radiation field; we have introduced a dimensionless dipole moment D for the interaction strength, with D^2 proportional to the laser beam intensity. The notation E stands for the quasienergy, in units of ω , of the two-level atom in the classical radiation field. It can also be directly called the energy level, if one treats the radiation as a quantum field. $\mathbf{Y} = (Y_1, Y_2)^t$, and σ_x and σ_z are Pauli matrices; I is the 2×2 unit matrix.

This equation is usually derived from the quantum-mechanical equations of motion for a two-level atom interacting with a classical, single-frequency mode in the *dipole* approximation. Below we will show that it can also be derived from the quantum-field approach in the large-photon-number (LPN) limit without any other approximation. For this reason, we regard the equations of motion (1) as an exact description of a driven two-level system when the driving field is a classical field.

Let us start from the equation of motion for a two-level atom interacting with a single-mode quantum field:

$$[\Delta \sigma_z + \omega N + |e|g \sigma_x (a + a^\dagger)] |\phi\rangle = -E |\phi\rangle, \quad (2)$$

which is equivalent to the one in Cohen-Tannoudji *et al.* [5], if we set $2\Delta = \omega_0$, $1/2 \sigma = \mathbf{J}$, $g = \lambda/4 |e|$, and $E = -E'$.

Now, we introduce a new basis $|y\rangle \equiv \sum_n y^n |n\rangle$ with $|n\rangle$ being Fock states:

$$|\phi\rangle \rightarrow \phi(y) \equiv \sum_n y^n \langle n | \phi \rangle. \quad (3)$$

Then, in the LPN limit, the equation of motion (2) becomes

$$\sum_n [\Delta \sigma_z y^n + n y^n \omega + |e| \Lambda \sigma_x (y^{n-1} + y^{n+1})] \phi_n = -E \sum_n y^n \phi_n, \quad (4)$$

where

$$\phi_n \equiv \langle n | \phi \rangle, \quad \Lambda \equiv g \sqrt{n}. \quad (5)$$

We further rewrite the above equation as

$$\left[\Delta \sigma_z + \omega y \frac{d}{dy} + |e| \Lambda \sigma_x (y^{-1} + y) \right] \phi(y) = -E \phi(y). \quad (6)$$

Letting

$$2|e|\Lambda \equiv D\omega, \quad y \equiv -e^{i\omega\tau}, \quad \omega = 1, \quad (7)$$

we obtain Eq. (1). Starting with Eq. (1) and going backward through the proof, with mapping y^n to Fock state $|n\rangle$ and resuming the commutation relation between y and y^{-1} , we

can recover Eq. (2). To recover ω , one should just take $\Delta \rightarrow \Delta/\omega$ and $E \rightarrow E/\omega$, with D remaining dimensionless.

III. SOLVING THE ALGEBRAIC EQUATIONS OF MOTION

Write the solutions in the case of $\Delta \neq 0$ in the form

$$\mathbf{Y} = C_1(\tau)\bar{\mathbf{Y}}^{(1)} + C_2(\tau)\bar{\mathbf{Y}}^{(2)}, \quad (8)$$

where $\bar{\mathbf{Y}}^{(1)}$ and $\bar{\mathbf{Y}}^{(2)}$ are two linearly independent solutions of Eq. (1) with $\Delta=0=E$:

$$\bar{\mathbf{Y}}^{(1)}(\tau) = e^{-iD \sin \tau} \frac{1}{\sqrt{2}}(1, -1)^t, \quad \bar{\mathbf{Y}}^{(2)}(\tau) = e^{iD \sin \tau} \frac{1}{\sqrt{2}}(1, 1)^t. \quad (9)$$

Here the superscript t means transposition. These solutions are orthonormal $\bar{\mathbf{Y}}^{(i)\dagger}\bar{\mathbf{Y}}^{(j)} = \delta_{ij}$, and satisfy

$$\bar{\mathbf{Y}}^{(1)\dagger}\sigma_z\bar{\mathbf{Y}}^{(1)} = \bar{\mathbf{Y}}^{(2)\dagger}\sigma_z\bar{\mathbf{Y}}^{(2)} = 0,$$

$$\bar{\mathbf{Y}}^{(1)\dagger}\sigma_z\bar{\mathbf{Y}}^{(2)} = (\bar{\mathbf{Y}}^{(2)\dagger}\sigma_z\bar{\mathbf{Y}}^{(1)})^* = e^{i2D \sin \tau}.$$

The resulting differential equations are

$$\begin{aligned} i\frac{d}{d\tau}C_1(\tau) - \Delta C_2(\tau)e^{i2D \sin \tau} - EC_1(\tau) &= 0, \\ i\frac{d}{d\tau}C_2(\tau) - \Delta C_1(\tau)e^{-i2D \sin \tau} - EC_2(\tau) &= 0. \end{aligned} \quad (10)$$

Using the expansions

$$C_1(\tau) = \sum_s C_{1s}e^{-is\tau}, \quad C_2(\tau) = \sum_s C_{2s}e^{-is\tau}, \quad (11)$$

Eqs. (10) can be transformed into a set of linear equations:

$$sC_{1s} - \Delta \sum_t C_{2t}J_{t-s}(2D) - EC_{1s} = 0,$$

$$sC_{2s} - \Delta \sum_t C_{1t}J_{t-s}(-2D) - EC_{2s} = 0, \quad (12)$$

where $J_n(x)$ are ordinary Bessel functions and s and t are integers running from $-\infty$ to ∞ . However, each of the equations involves an infinite sum of terms, so they are still complicated. To simplify them, we use the Bessel functions to construct a transformation:

$$A_q \equiv \sum_s C_{1s}J_{s-q}(-2D). \quad (13)$$

The inverse transformation is

$$C_{1s} = \sum_q A_q J_{q-s}(2D). \quad (14)$$

Using the inverse transformation to express Eq. (12) and the recurrence relations for the Bessel functions, $nJ_n(2D) = D[J_{n-1}(2D) + J_{n+1}(2D)]$, we obtain

$$\Delta C_{2s} = -D(A_{s+1} + A_{s-1}) + (s - E)A_s,$$

$$C_{2s} = \frac{\Delta}{s - E}A_s. \quad (15)$$

So finally the new variables A_s satisfy a set of simple linear equations

$$\frac{D(E-s)}{(E-s)^2 - \Delta^2}(A_{s+1} + A_{s-1}) + A_s = 0, \quad (16)$$

with $s = \dots, -2, -1, 0, 1, 2, \dots$. Each equation now involves only three terms. This success of simplification is crucial to our subsequent treatments.

IV. INFINITE DETERMINANT AND QUASIENERGIES

For a nontrivial solution to Eqs. (16) to exist, the quasienergy E has to be such that the following infinite determinant vanishes:

$$\det(E) = \begin{vmatrix} \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \alpha_{-2} & \beta_{-2}(E) & 0 & 0 & 0 & \cdots \\ \cdots & \gamma_{-1}(E) & \alpha_{-1} & \beta_{-1}(E) & 0 & 0 & \cdots \\ \cdots & 0 & \gamma_0(E) & \alpha_0 & \beta_0(E) & 0 & \cdots \\ \cdots & 0 & 0 & \gamma_1(E) & \alpha_1 & \beta_1(E) & \cdots \\ \cdots & 0 & 0 & 0 & \gamma_2(E) & \alpha_2 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{vmatrix}, \quad (17)$$

with

$$\alpha_s = 1, \quad \beta_s(E) = \gamma_s(E) = \frac{D(E-s)}{(E-s)^2 - \Delta^2}. \quad (18)$$

A determinant of this type is called tridiagonal, or it is called a continuant [13].

In the previous literature, this kind of infinite determinants was evaluated by using various approximations—e.g., the power series expansion in D [10]. Here we will evaluate this infinite determinant exactly, using techniques in complex analysis. The key observation is that the tridiagonal infinite determinant in Eq. (17) is absolutely convergent, since the infinite sum $\sum_s \beta_s \gamma_{s+1}$ is absolutely convergent. (See, for example, the classical treatise in [15].)

Therefore, if we regard the energy E as a complex variable, then the infinite determinant (17) defines an analytic function on the complex- E plane. Actually it is a meromorphic function of E which has two groups of poles at $E = \pm(\Delta + s)$, ($s = 0 \pm 1, \pm 2, \dots$).

When $2\Delta = n$ for integer $n \geq 1$, we call the case *preresonance*. In the nonpreresonant case where $2\Delta \neq n$, the poles of $\det(E)$ are all simple poles. Since $\beta_s(E)$ and $\gamma_s(E)$ are periodic functions of E with period unity, the poles in each group, $E = \pm(\Delta + s)$, respectively, are equally spaced and have the same residue. The residues

$$R_+ = \lim_{E \rightarrow \Delta \pm n} (E - \Delta \pm n) \det(E),$$

$$R_- = \lim_{E \rightarrow \Delta \pm n} (E + \Delta \pm n) \det(E) \quad (19)$$

are independent of n . Furthermore, it can be directly verified that the residues R_+ and R_- differ from each other only by a sign:

$$R_+(D, \Delta) = -R_-(D, \Delta). \quad (20)$$

Each group of poles with the same residue on the real E

axis of the complex- E plane suggests a cotangent function. We also observe that $\det(E = i\infty) = 1$. Thus the exact value of the determinant (17) can only be the following function:

$$\begin{aligned} \det(E) &= 1 + R_+ \sum_{n=-\infty}^{\infty} \left(\frac{1}{E - \Delta + n} - \frac{1}{E + \Delta + n} \right) \\ &= 1 + \pi R_+ \cot[\pi(E - \Delta)] - \pi R_+ \cot[\pi(E + \Delta)] \\ &= 1 + \pi R_+ \frac{\sin(2\pi\Delta)}{\sin[\pi(E - \Delta)] \sin[\pi(E + \Delta)]}. \end{aligned} \quad (21)$$

By the uniqueness theorem in complex analysis, the right side of Eq. (21) and that of Eq. (17) agree with each other on the whole E plane.

When 2Δ is a positive integer, the two groups of simple poles are merged to become double poles. When $\Delta = 0$, the poles at $E = \text{integer}$ still remain as first-order or zeroth-order ones. (The details will be discussed in the Appendix.)

Thus we are able to put the characteristic equation $\det(E) = 0$ into an exact and closed form

$$\sin[\pi(E - \Delta)] \sin[\pi(E + \Delta)] = -\pi R_+ \sin(2\pi\Delta). \quad (22)$$

Solving the above equation, with inclusion of the preresonance case, we obtain a cosine function of the quasienergy:

$$\begin{aligned} \cos(2\pi E) &= \cos(2\pi\Delta) + 2\pi R_+ \sin(2\pi\Delta) \quad (2\Delta \neq n), \\ \cos(2\pi E) &= \cos(2\pi\Delta) + (-1)^n 2\pi^2 r_n \quad (2\Delta = n), \end{aligned} \quad (23)$$

where r_n are residues of R_+ as a function of 2Δ , defined by the limiting processes

$$\lim_{2\Delta \rightarrow n} R_+ \sin(2\pi\Delta) = (-1)^n \lim_{2\Delta \rightarrow n} R_+ \pi(2\Delta - n) = (-1)^n \pi r_n. \quad (24)$$

We note that $r_0 = 0$ for $n = 0$. (The detailed proof is presented in the Appendix.)

This expression (23) for the energy shift has a unique advantage: the Floquet condition is automatically satisfied in view of the cosine function.

The next main job is to evaluate the factor R_+ . In the context below, for writing convenience, we use finite determinant notation to express the infinite determinants. We find

$$R_+ = \lim_{E \rightarrow \Delta} (E - \Delta) \det(E) = \begin{vmatrix} 1 & \frac{D(\Delta + 3)}{3(2\Delta + 3)} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \frac{D(\Delta + 2)}{2(2\Delta + 2)} & 1 & \frac{D(\Delta + 2)}{2(2\Delta + 2)} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{D(\Delta + 1)}{(2\Delta + 1)} & 1 & \frac{D(\Delta + 1)}{(2\Delta + 1)} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \frac{D(\Delta - 1)}{-1(2\Delta - 1)} & 1 & \frac{D(\Delta - 1)}{-1(2\Delta - 1)} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{D(\Delta - 2)}{-2(2\Delta - 2)} & 1 & \frac{D(\Delta - 2)}{-2(2\Delta - 2)} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \frac{D(\Delta - 3)}{-3(2\Delta - 3)} & 1 \end{vmatrix} \quad (25)$$

The following lemma is useful to determine the residues of R_+ .

Lemma. For any integer n , the function $\det(E)$ with $2\Delta = n$ has the second-order poles at $E = l + n/2$, where l is an arbitrary integer, with coefficients equal to the residue of $R_+(2\Delta)$ at the first-order pole $2\Delta = n$ —i.e.,

$$\lim_{E \rightarrow (l+n/2)} [E - (l + n/2)]^2 \det(E) \Big|_{2\Delta=n} = r_n, \quad (26)$$

where r_n are residue of the function $R_+(2\Delta)$ at the pole $2\Delta = n$.

Proof. From Eqs. (21) and (24),

$$\begin{aligned} \det(E) \Big|_{2\Delta=n} &= 1 + \frac{(-1)^n \pi^2 r_n}{\sin[\pi(E - \Delta)] \sin[\pi(E + \Delta)]} \Big|_{2\Delta=n} \\ &= 1 + \frac{\pi^2 r_n}{\sin^2[\pi(E - n/2)]}, \end{aligned} \quad (27)$$

we can see that when $E \rightarrow (l + n/2)$, the function

$\pi^2 / \sin^2[\pi(E - n/2)]$ behaves like a second-order pole $[E - (l + n/2)]^{-2}$.

In the $n=0$ case, the above proof still holds, since $R_+ \Big|_{2\Delta=0} = 0$ (see the Appendix) and $r_0=0$. Q.E.D.

From this lemma we learn that the function of $R_+(2\Delta)$ can only have first-order poles at nonzero integers. Thus, R_+ can be expressed as

$$R_+ = R_+^\infty + \sum_{n=-\infty}^{\infty} \frac{r_n}{2\Delta - n} = \sum_{n=1}^{\infty} \frac{4\Delta}{4\Delta^2 - n^2} r_n, \quad (28)$$

where (a) $r_n = r_{-n}$, (b) $r_0=0$, and (c) $R_+^\infty=0$ have been used. The proofs for (b) and (c) are given in the Appendix . The proof for (a) is the following: Using Eq. (26) to express r_{-n} , we verify that the values of the two factors on the left-hand side of this equation do not change with changing $n \rightarrow -n$. That the second factor does not change can be seen from Eqs. (21) and (20) while the first one can be seen with substituting l in $l - n/2$ by $l' + n$ since both l and l' can be arbitrary integers.

Further evaluation of R_+ is based on the evaluation of the residues r_n . In the following, we list a few low-photon-number residues as examples:

$$r_1 = \begin{pmatrix} 1 & \frac{7}{2}D & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ & \frac{3 \times 4}{2 \times 3} & & & & & & \\ \frac{5}{2}D & 1 & \frac{5}{2}D & \cdot & \cdot & \cdot & \cdot & \cdot \\ & & \frac{2 \times 3}{1 \times 2} & & & & & \\ \cdot & \frac{3}{2}D & 1 & \frac{3}{2}D & \cdot & \cdot & \cdot & \cdot \\ & & & \frac{1 \times 2}{D} & 0 & \frac{D}{2} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & -\frac{3}{2}D & 1 & -\frac{3}{2}D & \cdot \\ & & & & & -\frac{5}{2}D & 1 & -\frac{5}{2}D \\ \cdot & \cdot & \cdot & \cdot & \cdot & -\frac{3 \times 2}{4 \times 3} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -\frac{7}{2}D & 1 \\ & & & & & & & -\frac{4 \times 3}{\cdot} \end{pmatrix}, \tag{29}$$

$$r_2 = \begin{pmatrix} 1 & \frac{4D}{3 \times 5} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ & \frac{2 \times 4}{2 \times 4} & 1 & \frac{3D}{2 \times 4} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{2D}{1 \times 3} & 1 & \frac{2D}{1 \times 3} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 0 & 1 & 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & -\frac{2D}{3 \times 1} & 1 & -\frac{2D}{3 \times 1} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -\frac{3D}{4 \times 2} & 1 & -\frac{3D}{4 \times 2} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -\frac{4D}{5 \times 3} & 1 \end{pmatrix}, \tag{30}$$

$$r_3 = \begin{vmatrix} 1 & \frac{D\frac{7}{2}}{5 \times 2} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \frac{D\frac{5}{2}}{4 \times 1} & 1 & \frac{D\frac{5}{2}}{4 \times 1} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{D\frac{1}{2}}{2(-1)} & 1 & \frac{D\frac{1}{2}}{2(-1)} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \frac{D\left(-\frac{1}{2}\right)}{1(-2)} & 1 & \frac{D\left(-\frac{1}{2}\right)}{1 \times (-2)} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \frac{D\left(-\frac{5}{2}\right)}{(-1)(-4)} & 1 & \frac{D\left(-\frac{5}{2}\right)}{(-1)(-4)} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{D\left(-\frac{7}{2}\right)}{(-2)(-5)} & 1 & \cdot \end{vmatrix}, \tag{31}$$

and

$$r_4 = \begin{vmatrix} 1 & \frac{D4}{6 \times 2} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \frac{D3}{5 \times 1} & 1 & \frac{D3}{5 \times 1} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{D1}{3(-1)} & 1 & \frac{D1}{3(-1)} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 0 & 1 & 0 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{D(-1)}{1(-3)} & 1 & \frac{D(-1)}{1(-3)} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{D(-3)}{(-1)(-5)} & 1 & \frac{D(-3)}{(-1)(-5)} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{D(-4)}{(-2)(-6)} & 1 \end{vmatrix}. \tag{32}$$

For general n , r_n can be expressed as an determinant of infinite rank:

$r_n =$

$$\begin{array}{cccccccc}
 1 & \frac{D\left(\frac{n}{2}+3\right)}{3(n+3)} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \frac{D\left(\frac{n}{2}+2\right)}{2(n+2)} & 1 & \frac{D\left(\frac{n}{2}+2\right)}{2(n+2)} & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \frac{D\left(\frac{n}{2}+1\right)}{1(n+1)} & 1 & \frac{D\left(\frac{n}{2}+1\right)}{1(n+1)} & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \frac{D\left(\frac{n}{2}-1\right)}{-1(n-1)} & 1 & \frac{D\left(\frac{n}{2}-1\right)}{-1(n-1)} & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \frac{D\left(\frac{n}{2}-2\right)}{-2(n-2)} & 1 & \frac{D\left(\frac{n}{2}-2\right)}{-2(n-2)} & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \frac{D\left(\frac{n}{2}-3\right)}{-3(n-3)} & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 1 & \frac{D\left(\frac{n}{2}-3\right)}{3(n-3)} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \frac{D\left(\frac{n}{2}-2\right)}{2(n-2)} & 1 & \frac{D\left(\frac{n}{2}-2\right)}{2(n-2)} & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \frac{D\left(\frac{n}{2}-1\right)}{1(n-1)} & 1 & \frac{D\left(\frac{n}{2}-1\right)}{1(n-1)} & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \frac{D\left(\frac{n}{2}+1\right)}{-1(n+1)} & 1 & \frac{D\left(\frac{n}{2}+1\right)}{-1(n+1)} & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \frac{D\left(\frac{n}{2}+2\right)}{-2(n+2)} & 1 & \frac{D\left(\frac{n}{2}+2\right)}{-2(n+2)} & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \frac{D\left(\frac{n}{2}+3\right)}{-3(n+3)} & 1 & \cdot
 \end{array}$$

(33)

In this notation, the lower part in the expression is the continuation of the upper part in the direction of the main diagonal.

We have been able to work out the first a few terms for the residues in the dipole expansion. Here we only cite the results:

$$\begin{aligned} r_1 &= -\frac{1}{4}D^2 + \left(\frac{\pi^2}{48} + \frac{1}{64}\right)D^4 + \dots, \\ r_2 &= -\frac{1}{9}D^4 + \frac{13}{162}D^6 + \dots, \\ r_n &= -\frac{1}{4}\left(\frac{n}{n^2-1}\right)^2 D^4 + \dots \quad (n \neq 1), \end{aligned} \quad (34)$$

The numerical coefficients given here are all exact.

Thus, the expression for R_+ up to the D^4 term is

$$\begin{aligned} R_+ &= \left[-\frac{D^2}{4} + D^4\left(\frac{\pi^2}{48} + \frac{1}{64}\right) + \dots \right] \frac{4\Delta}{4\Delta^2-1} \\ &+ \sum_{n=2}^{\infty} \left[-\frac{D^4}{4}\left(\frac{n}{n^2-1}\right)^2 + \dots \right] \frac{4\Delta}{4\Delta^2-n^2}. \end{aligned} \quad (35)$$

The explicit form of R_+ can be used to evaluate the energy shift. In the preresonance case, from Eq. (23), the cosine energy shift reads as

$$\cos(2\pi E) = -1 + \frac{\pi^2}{2}D^2 - \pi^2\left(\frac{\pi^2}{24} + \frac{1}{32}\right)D^4 + \dots \quad (2\Delta = 1),$$

$$\begin{aligned} \cos(2\pi E) &= (-1)^n - (-1)^n \frac{\pi^2}{2}\left(\frac{n}{n^2-1}\right)^2 D^4 + \dots \\ (2\Delta &= n \neq 1). \end{aligned} \quad (36)$$

There are many exact ways to express E as an exact function of Δ . The following are the suggested ones:

$$\begin{aligned} E &= \frac{1}{\pi} \cos^{-1} \sqrt{\cos^2(\pi\Delta) + \pi R_+ \sin(2\pi\Delta)} \quad (2\Delta \neq n), \\ E &= \frac{1}{\pi} \cos^{-1}(\pi\sqrt{-r_{2k+1}}) \quad (2\Delta = 2k+1) \end{aligned} \quad (37)$$

and

$$\begin{aligned} E &= \frac{1}{\pi} \sin^{-1} \sqrt{\sin^2(\pi\Delta) - \pi R_+ \sin(2\pi\Delta)} \quad (2\Delta \neq n), \\ E &= \frac{1}{\pi} \sin^{-1}(\pi\sqrt{-r_{2k}}) \quad (2\Delta = 2k). \end{aligned} \quad (38)$$

The right side of the equations can all be added with an integer, due to the Floquet feature for quasienergy. Here we leave the sign determination for the square roots to the Discussion section.

The Bloch-Siegert shift, defined as $E_{BS} = 2E - 2\Delta$, has now the exact expressions

$$\begin{aligned} E_{BS} &= \frac{2}{\pi} \cos^{-1} \sqrt{\cos^2(\pi\Delta) + \pi R_+ \sin(2\pi\Delta)} - 2\Delta \quad (2\Delta \neq n), \\ E_{BS} &= \frac{2}{\pi} \cos^{-1}(\pi\sqrt{-r_{2k+1}}) - 2\Delta \quad (2\Delta = 2k+1) \end{aligned} \quad (39)$$

and

$$\begin{aligned} E_{BS} &= \frac{2}{\pi} \sin^{-1} \sqrt{\sin^2(\pi\Delta) - \pi R_+ \sin(2\pi\Delta)} - 2\Delta \quad (2\Delta \neq n), \\ E_{BS} &= \frac{2}{\pi} \sin^{-1}(\pi\sqrt{-r_{2k}}) - 2\Delta \quad (2\Delta = 2k). \end{aligned} \quad (40)$$

V. WAVE FUNCTIONS

Equation (16) can be further written as [14]

$$\text{for } s > 0, \quad \frac{A_s}{A_{s-1}} = \frac{-1}{\frac{(E-s)^2 - \Delta^2}{D(E-s)} + \frac{A_{s+1}}{A_s}}, \quad (41)$$

$$\text{for } s < 0, \quad \frac{A_s}{A_{s+1}} = \frac{-1}{\frac{(E-s)^2 - \Delta^2}{D(E-s)} + \frac{A_{s-1}}{A_s}}, \quad (42)$$

$$\text{for } s = 0, \quad \frac{A_{-1}}{A_0} + \frac{E^2 - \Delta^2}{DE} + \frac{A_1}{A_0} = 0. \quad (43)$$

By iterating the first relation, we express A_1/A_0 as a continued fraction:

$$\frac{A_1}{A_0} = -\frac{1}{\frac{(E-1)^2 - \Delta^2}{D(E-1)} - \frac{1}{\frac{(E-2)^2 - \Delta^2}{D(E-2)} - \dots}}. \quad (44)$$

Similarly by iterating the second relation, we have

$$\frac{A_{-1}}{A_0} = -\frac{1}{\frac{(E+1)^2 - \Delta^2}{D(E+1)} - \frac{1}{\frac{(E+2)^2 - \Delta^2}{D(E+2)} - \dots}}. \quad (45)$$

Putting back all the transformations made, we obtain

$$\begin{aligned} \mathbf{Y}^\mp &= \sum_s \sum_q A_q^\mp \mathbf{J}_{q-s}(2D) e^{-is\tau} \bar{\mathbf{Y}}^{(1)} + \sum_s \frac{\Delta}{s \pm E} A_s^\mp e^{-is\tau} \bar{\mathbf{Y}}^{(2)} \\ &= \sum_s A_s^\mp e^{-is\tau} e^{i2D \sin \tau} \bar{\mathbf{Y}}^{(1)} + \sum_s \frac{\Delta}{s \pm E} A_s^\mp e^{-is\tau} \bar{\mathbf{Y}}^{(2)} \\ &= \sum_s A_s^\mp e^{-is\tau} e^{i2D \sin \tau} e^{-iD \sin \tau} \frac{1}{\sqrt{2}} (1, -1)^t \\ &+ \sum_s \frac{\Delta}{s \pm E} A_s^\mp e^{-is\tau} e^{iD \sin \tau} \frac{1}{\sqrt{2}} (1, 1)^t \end{aligned}$$

$$\begin{aligned}
 &= \sum_s A_s^\mp e^{-is\tau} \frac{1}{\sqrt{2}} \left[(1, -1)^t + \frac{\Delta}{s \pm E} (1, 1)^t \right] e^{iD \sin \tau} \\
 &= e^{iD \sin \tau} \sum_s A_s^\mp e^{-is\tau} \frac{1}{\sqrt{2}} \left(\frac{\Delta}{s \pm E} + 1, \frac{\Delta}{s \pm E} - 1 \right)^t, \quad (46)
 \end{aligned}$$

where the superscript \mp denotes that the solutions correspond to $\mp E$.

VI. FREEMAN RESONANCES

In our solutions, we identify a Freeman resonance when the new energy spacing $2E$, which is field-intensity dependent, is an integral multiple of the field photon energy. The derived wave functions apparently have singularities only at $2E = 2s\hbar\omega$ ($s=0, \pm 1, \pm 2, \pm 3, \dots$), and not at the preresonance case. Here we do not exclude the $2E=0$ case, since $2E=0$ means $2E$ can be any integer. We also see from the wave function that in the preresonance case, the wave functions are finite, as well as the quasienergies given by Eqs. (37) and (38).

All this means that the preresonances are not true resonances; only Freeman resonances are true resonances. At first glance, one may think that the Freeman resonances occur only when the resonating photon number is an even number. Since the quasienergy spacing $2E$ can be added with an arbitrary integral multiple of the photon energy, we can replace $2E' = 2E + 1$ in the above equations related to the wave functions. Thus, we immediately find the resonances with odd photon numbers. This analysis also indicates that we need four or more different quasienergy levels as basic ones even in the nonresonance case, since $2E' = 2E + 1$ may give different wave functions. On the other hand, we do not need more than four as basic ones, since $2E' = 2E + 2$ will not give a new wave function and it is included in the iteration process in the continued fractions. Thus, we conclude that we need four and only four different quasienergies as basic ones to produce the wave functions.

At the Freeman resonances where $2E = n$, the intensity of the field and the original energy spacing 2Δ satisfy the following equation from Eq. (23):

$$\cos(2\pi\Delta) + 2\pi R_+ \sin(2\pi\Delta) = (-1)^n. \quad (47)$$

When $n = \text{odd}$, the equation reduces to

$$2\pi R_+ = -\cot(\pi\Delta). \quad (48)$$

When $n = \text{even}$, the equation reduces to

$$2\pi R_+ = \tan(\pi\Delta). \quad (49)$$

In this case, as we pointed out before, the wave functions have an infinite amplitude.

Equations (48) and (49) are transcendental equations. For a given field intensity and Freeman resonance ($E = n\omega$), one can solve the transcendental equation to identify the resonating atomic level, which has the original spacing 2Δ from the ground state. This equation has discrete solutions for 2Δ ,

which change when the field intensity changes. This theoretical feature does agree with experimental findings. Experimentalists call an electron energy peak in an ATI spectrum a Freeman resonance when the energy spacing between the ground state and the energy peak is an integral multiple of the laser photon energy and interpret the energy peak as a formation of photoelectrons from a shifted Rydberg state. ATI spectra do show that the Freeman resonances have a discrete feature for a fixed laser intensity. When the laser intensity changes, different sets of Rydberg levels come into play consecutively as Freeman resonances appearing in the ATI spectrum.

VII. DISCUSSION

The basic requirement to a correct solution of an interacting system is when the interaction vanishes, the solution reduces to the one of the corresponding non interacting system. For the problem at hand, the interaction is imposed through the dipole moment D . Thus the leading term of quasienergy in the expansion in powers of $D^2\omega^2$ should satisfy the basic requirement and also should signify the physical meaning of the field intensity. Another important quantity is $(2\Delta - \omega)^2$ which signifies the detuning of the field frequency from the transition frequency of the original two-level atom and competes with $D^2\omega^2$ in the near-preresonance processes. To see the interesting competition in different limiting processes, we consider the following two cases, respectively.

A. Energy shift at exact n -photon pre resonances

Practically, if we can tune up a laser in a way that an integral multiple of laser frequency $n\omega$ matches the energy spacing 2Δ of a two-level atom—i.e., $(2\Delta - n\omega)^2 \ll D^2\omega^2$ —we can set $2\Delta = n\omega$ and use Eqs. (36)–(40) to obtain the energy shift in the small-dipole limit.

We have the following three subcases

1. Single-photon case

In the single-photon preresonance case, the quasienergy E has a simple form by just keeping the leading term of D , with ω recovered in the expression explicitly,

$$E = \frac{\omega}{\pi} \cos^{-1} \left(\pm \frac{\pi D}{2} \right). \quad (50)$$

Using $\cos^{-1}(x+d) = \cos^{-1}x - (1-x^2)^{-1/2}d$, where $x=0$ and $d = \pm \pi D/2$, we find

$$E = \frac{\omega}{2}(1 + D), \quad E_{BS} = \omega D, \quad (51)$$

where the negative sign in Eq. (50) is selected according to the limiting process from the near-preresonance case in the next subsection.

This is a simple interesting result that the shift is proportional to D .

2. Odd-number photon case ($n \neq 1$)

In this case, the quasienergy is

$$E = \frac{\omega}{\pi} \cos^{-1} \left(\pm \frac{\pi D^2}{2} \frac{n}{n^2 - 1} \right). \quad (52)$$

Using $\cos^{-1}(x+d) = \cos^{-1}x - (1-x^2)^{-1/2}d$, where $x=0$ and $d = \pm n\pi D^2/2(n^2-1)$, we find

$$E = \frac{n\omega}{2} \left(1 + \frac{D^2}{n^2 - 1} \right), \quad E_{BS} = \frac{n\omega D^2}{n^2 - 1}, \quad (53)$$

with the same negative sign selected as above.

3. Even-number photon case

In this case, the quasienergy is

$$E = \frac{\omega}{\pi} \sin^{-1} \left(\pm \frac{\pi D^2}{2} \frac{n}{n^2 - 1} \right). \quad (54)$$

Using $\sin^{-1}(x+d) = \sin^{-1}x + (1-x^2)^{-1/2}d$, where $x=0$ and $d = \pm n\pi D^2/2(n^2-1)$, we find

$$E = \frac{n\omega}{2} \left(1 + \frac{D^2}{n^2 - 1} \right), \quad E_{BS} = \frac{n\omega D^2}{n^2 - 1}, \quad (55)$$

where the positive sign is selected in Eq. (54) according to the same limiting process as discussed above.

Now we see that the BS shift is proportional to D in the single-photon preresonance case, while it is proportional to D^2 in the multiphoton preresonance case.

B. Energy shift in the weak-field and near-preresonance case

In the previous case, we let $(2\Delta - n\omega)^2$ be infinitesimal first. In the present case, switching the limiting procedures we let $D^2\omega^2$ be infinitesimal first—i.e., $D^2\omega^2 \ll (2\Delta - n\omega)^2$.

To treat this case, we need to expand the term $2\pi \sin(2\pi\Delta)R_+$ in Eq. (23) as

$$\begin{aligned} & 2\pi \sin(2\pi\Delta) \sum_{j=1}^{\infty} \left(\frac{1}{2\Delta - j} + \frac{1}{2\Delta + j} \right) r_j \\ & \approx (-1)^n 2\pi^2 \left\{ r_n - (2\Delta - n)^2 \frac{\pi^2}{6} r_n \right. \\ & + (2\Delta - n) \left(\sum_{j \geq 1, j \neq n} \frac{1}{n-j} + \sum_{j=1}^{\infty} \frac{1}{n+j} \right) r_j \\ & - (2\Delta - n)^2 \\ & \left. \times \left[\sum_{j \geq 1, j \neq n} \frac{1}{(n-j)^2} + \sum_{j=1}^{\infty} \frac{1}{(n+j)^2} \right] r_j \right\}. \quad (56) \end{aligned}$$

We consider the following subcases

1. Single-photon case

In the small-dipole case we only keep r_1 , because only r_1 has D^2 as its leading order, while all other r_n have D^4 as their leading order. Thus, from Eqs. (23) and (28), the cosine energy relation reads

$$\cos \left(2\pi \frac{E}{\omega} \right) = -1 + \frac{\pi^2}{2} \left(\frac{2\Delta}{\omega} - 1 \right)^2 - 2\pi^2 r_1 - \pi^2 r_1 \left(\frac{2\Delta}{\omega} - 1 \right), \quad (57)$$

where $r_1 \approx -D^2/4$ in the leading order. By expanding $\cos(2\pi E/\omega) \approx -1 + \pi^2[(2E/\omega) - 1]^2/2$, we obtain an approximated quadratic equation

$$(2E - \omega)^2 = (2\Delta - \omega)^2 + D^2\omega^2 + \frac{D^2}{2}\omega(2\Delta - \omega), \quad (58)$$

which has the solution

$$\begin{aligned} E_{BS} & \equiv (2E - 2\Delta) \\ & = -(2\Delta - \omega) \\ & \pm \sqrt{(2\Delta - \omega)^2 + D^2\omega^2 + \frac{D^2}{2}\omega(2\Delta - \omega)}. \quad (59) \end{aligned}$$

This result agrees with the one from the RWA but with an extra correction term, the last term underneath the square-root symbol.

For a small dipole $D^2 \ll 1$, choosing the positive sign, the BS shift reduces to

$$E_{BS} \approx \frac{D^2\omega^2}{2(2\Delta - \omega)} + \frac{1}{4}D^2\omega. \quad (60)$$

The extra term, the last term in the above equation, signifies the one-photon emission effect beyond the RWA. Here we see that when $D^2\omega^2 \ll (2\Delta - \omega)^2$ —i.e., the interaction term is smaller than the detuning—the BS shift is proportional to D^2 .

The sign selection here is forced by the requirement that when the interaction $D\omega \rightarrow 0$, the value of E_{BS} has to vanish. With the positive sign selected in Eq. (59), letting $(2\Delta - \omega) \rightarrow 0$ directly, we get the same result as Eq. (51), whose sign is thus determined.

2. Multiphoton case

We have the expansion

$$\begin{aligned} \cos \left(2\pi \frac{E}{\omega} \right) & = (-1)^n \left\{ 1 - \frac{\pi^2}{2} \left(\frac{2\Delta}{\omega} - n \right)^2 \right\} + (-1)^n 2\pi^2 \left(\frac{1}{n-1} \right. \\ & \left. + \frac{1}{n+1} \right) \left(\frac{2\Delta}{\omega} - n \right) r_1. \quad (61) \end{aligned}$$

By expanding $\cos(2\pi E/\omega) \approx (-1)^n \{1 - \pi^2 [(2E/\omega) - n]^2/2\}$, we obtain an approximate quadratic equation

$$(2E - n\omega)^2 = (2\Delta - n\omega)^2 + D^2 \omega \frac{2n}{n^2 - 1} (2\Delta - n\omega), \quad (62)$$

which has the solution

$$E_{BS} \equiv (2E - 2\Delta) = D^2 \omega \frac{n}{n^2 - 1}, \quad (63)$$

where the sign is determined by the same method as before, which also justifies the sign selection in Eqs. (53) and (55). An amazing thing here is that in the two different limiting processes and with different formulas, E_{BS} behaves the same way, both proportional to D^2 and with the same proportionality constant.

VIII. CONCLUSIONS

In the following we summarize the features of the exact solution obtained

(i) It explicitly exhibits the Floquet quasienergy behavior; namely, the quasienergy spacing is determined only up to its cosine.

(ii) It incorporates all multiphoton effects.

(iii) When the original energy spacing matches an integer number of photon energy, the preresonance case, the interacting system does not really resonate. Both quasienergies and wave functions are finite.

(iv) We have shown theoretically that when the shifted energy spacing matches an integer number of photon energy, the interacting system resonates. This theoretical feature explains the Freeman resonances observed in ATI experiments. We have also proved that the Freeman resonances have a discrete feature, and when the field intensity changes different sets of unoccupied, excited atomic levels come into play as the resonances.

(v) The Bloch-Siegert shift vanishes when the interaction D vanishes. The way it vanishes obeys some simple rules: Near the single-photon preresonance, whether the BS shift vanishes as D or D^2 depends on whether the detuning first goes to zero or the interaction strength first goes to zero. Near the multiphoton preresonances, the BS shift always vanishes as D^2 , independent of the limiting process. These rules can be subject to experimental tests.

ACKNOWLEDGMENTS

D.S.G. was supported in part by a summer grant of the Physics Department of Ohio State University. Y.S.W. was supported in part by the NSF through Grant Nos. PHY-9970701 and PHY-0457018. The authors thank R. R. Freeman and J. Gao for helpful discussions.

APPENDIX

We will show that R_+ as the residue of $\det(E)$ vanishes when $2\Delta=0$ and that

$$R_+^\infty = \lim_{\Delta \rightarrow \infty} R_+ = \begin{vmatrix} 1 & \frac{D}{3 \times 2} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \frac{D}{2 \times 2} & 1 & \frac{D}{2 \times 2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{D}{1 \times 2} & 1 & \frac{D}{1 \times 2} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \frac{D}{-1 \times 2} & 1 & \frac{D}{-1 \times 2} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{D}{-2 \times 2} & 1 & \frac{D}{-2 \times 2} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \frac{D}{-3 \times 2} & 1 \end{vmatrix} = 0. \quad (A1)$$

In the case of $2\Delta=0$,

$$\det(E)|_{\Delta=0} = \begin{vmatrix} 1 & \frac{D}{E+3} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \frac{D}{E+2} & 1 & \frac{D}{E+2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{D}{E+1} & 1 & \frac{D}{E+1} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{D}{E} & 1 & \frac{D}{E} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \frac{D}{E-1} & 1 & \frac{D}{E-1} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{D}{E-2} & 1 & \frac{D}{E-2} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \frac{D}{E-3} & 1 \end{vmatrix}. \tag{A2}$$

We notice

$$\lim_{E \rightarrow n} (E - n) \det(E)|_{\Delta=0} = R_+(\Delta = 0), \tag{A3}$$

$$-\frac{x}{2n}(J_{n-1} + J_{n+1}) + J_n = 0,$$

which does not depend on n : thus,

$$\det(E)|_{\Delta=0} = 1 + \pi R_+(\Delta = 0) \cot(\pi E). \tag{A4}$$

$$K(J_{-1} + J_1) = 0, \tag{A8}$$

The characteristic equation is obtained by setting $\det(E)|_{\Delta=0} = 0$ —i.e.,

$$\sin(\pi E) + \pi R_+(\Delta = 0) \cos(\pi E) = 0, \tag{A5}$$

where K is an arbitrary constant.

Let n run from $-\infty$ to ∞ . The algebraic equation set for J_n has nonzero solutions. So the coefficient determinant must be zero—i.e.,

which has the solution

$$E = -\frac{1}{\pi} \tan^{-1}[\pi R_+(\Delta = 0)], \tag{A6}$$

where $R_+(\Delta = 0)$ is

$$R_+(\Delta = 0) = \begin{vmatrix} 1 & \frac{D}{3} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \frac{D}{2} & 1 & \frac{D}{2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & D & 1 & D & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{D}{2} & 0 & \frac{D}{2} & \cdot & \cdot \\ \cdot & \cdot & \cdot & -\frac{D}{1} & 1 & -\frac{D}{1} & \cdot \\ \cdot & \cdot & \cdot & \cdot & -\frac{D}{2} & 1 & -\frac{D}{2} \\ \cdot & \cdot & \cdot & \cdot & \cdot & -\frac{D}{3} & 1 \end{vmatrix} = 0. \tag{A7}$$

$$\det(x) = \begin{vmatrix} 1 & \frac{-x}{6} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \frac{-x}{4} & 1 & \frac{-x}{4} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{-x}{2} & 1 & \frac{-x}{2} & \cdot & \cdot & \cdot \\ \cdot & \cdot & K & 0 & K & \cdot & \cdot \\ \cdot & \cdot & \cdot & \frac{x}{2} & 1 & \frac{x}{2} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{x}{4} & 1 & \frac{x}{4} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \frac{x}{6} & 1 \end{vmatrix} = 0. \tag{A9}$$

The last step ($=0$) needs a proof.

Proof. We use a recurrence relation of Bessel functions

By setting $x = -D$ and $K = D/2$ we get Eq. (A1). By setting $x = -2D$ and $K = D/2$ we get Eq. (A7). Q.E.D. From $R_r(\Delta = 0) = 0$, we immediately reach $r_0 = 0$.

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